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ECURITY CLASSIFIC **AD-A236 871**

JMENTATION PAGE

a. REPORT SECUR Unclassified	1b. RESTRICTIVE MARKINGS N/A
2a. SECURITY CLASSIFICATION AUTHORITY N/A	3. DISTRIBUTION / AVAILABILITY OF REPORT Approved for public release; distribution unlimited.
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE N/A	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) N00014-90-J-1119-10	5. MONITORING ORGANIZATION REPORT NUMBER(S)
6a. NAME OF PERFORMING ORGANIZATION Board of Regents of the University of Wisconsin-Madison / 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION Office of Naval Research Branch Office Chicago
6c. ADDRESS (City, State, and ZIP Code) 750 University Avenue Madison, WI 53706	7b. ADDRESS (City, State, and ZIP Code) 536 S. Clark Street Chicago, IL 60605
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Office of Naval Research--Chemistry Program / 8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER N00014-90-J-1119-10
8c. ADDRESS (City, State, and ZIP Code) 800 N. Quincy Street Arlington, VA 22217	10. SOURCE OF FUNDING NUMBERS: PROGRAM ELEMENT NO. / PROJECT NO. / TASK NO. / WORK UNIT ACCESSION NO

11. TITLE (Include Security Classification)
DIFFRACTION DETERMINATION OF THE STRUCTURE OF METASTABLE THREE-DIMENSIONAL CRYSTALS OF Ge GROWN ON Si(001)

12. PERSONAL AUTHOR(S)
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13a. TYPE OF REPORT	13b. TIME COVERED FROM ____ TO ____	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
		May 25, 1991	12

16. SUPPLEMENTARY NOTATION
Appl. Phys. Letters, in press

17. COSATI CODES: FIELD	GROUP	SUB-GROUP

18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
Growth, structure, surfaces, Ge on Si(001) scanning tunneling microscopy, diffraction

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

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20 DISTRIBUTION / AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ OTIC USERS	Unclassified
22a NAME OF RESPONSIBLE INDIVIDUAL Max G. Lagally	22b. TELEPHONE (Include Area Code) 608-263-2078 / 22c. OFFICE SYMBOL

DD FORM 1473, 84 MAR 83 APR edition may be used until exhausted. SECURITY CLASSIFICATION OF THIS PAGE

OFFICE OF NAVAL RESEARCH

Contract No.: N00014-90-J-1119

R&T Code: 413f008

TECHNICAL REPORT NO. 10

Diffraction Determination of the Structure of Metastable Three-Dimensional Crystals of Ge Grown On Si(001)

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May 25, 1991

Appl. Phys. Letters, in press

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ABSTRACT

A straightforward kinematic analysis of diffraction from metastable three-dimensional crystallites of Ge grown on Si(001) is presented. Low-energy electron diffraction data from these crystallites agree with diffraction images calculated for a structure determined from scanning-tunneling microscopy data. Additionally, reflection high-energy electron diffraction images predicted for these crystals agree with existing data.

Introduction

Recent scanning tunneling microscopy (STM) measurements of the growth of Ge on Si(001) have revealed metastable Ge crystallites that form on top of the initial ∿ three-monolayer two-dimensional Ge phase.[1] Figure 1 is an STM scan of one of these metastable "hut" clusters, showing its well-defined facet structure. Each crystallite consists of a pyramid or elongated pyramid with four equivalent facets. The facets were proposed[1], on the basis of detailed STM scans, to be reconstructed {105} planes consisting of (001) terraces separated by monatomic-height steps running parallel to <100> directions. Each terrace is two dimer pairs wide with the dimer pairs angled 45° with respect to the step and rotating 90° upon crossing a step. Alternatively, a facet can be described as a vicinal (001) surface having a miscut of 11.3° toward <100>.

We have also observed this phase using low-energy electron diffraction (LEED). Diffraction patterns of Si(001) with and without the Ge hut crystals present are shown in Fig. 2. The Ge huts add extra features about the substrate beams that look like X's. These diffraction patterns are relatively straightforward to interpret in terms of the structure causing them. Vicinal surfaces are well known to cause a splitting of diffracted beams in a direction normal to the steps[2]. Because the extra spots in Fig. 2b are split in a direction 45° relative to the symmetry of the substrate reflections (i.e., the substrate unit mesh has sides parallel to

<110>) it is immediately known that the facets must have <100>-type zone axes, i.e., steps parallel to <100> as in the model established by STM.[1] The diffraction pattern in Fig. 2b can be reproduced via a kinematic calculation for the unit mesh proposed in Ref. 1. Taking the dimer pairs from odd-and even-level terraces to scatter equivalently yields the structure factor:

$$F = \cos(\vec{S}\cdot(\hat{j}-\hat{i})a/4) + \cos(\vec{S}\cdot(\hat{i}+\hat{j})a/4)e^{i\vec{S}\cdot\vec{c}}, \qquad (1)$$

where the basis vector $\vec{c} = 5a\hat{i}/4 + 3a\hat{j}/4 - a\hat{k}/4$, $a = 5.66\text{Å}$ is the bulk lattice constant for Ge, and $\vec{S}$ is a reciprocal-lattice vector. The scattered intensity from this (105) facet is then:

$$I = \left| F \sum_{n}^{N} e^{in\vec{S}\cdot\vec{a}} \sum_{m}^{M} e^{im\vec{S}\cdot\vec{b}} \right|^2 \qquad (2)$$

with unit mesh vectors $\vec{a} = 5a\hat{i}/2 - a\hat{k}/2$, $\vec{b} = 2a\hat{j}$ and n,m integers. For simplicity the facets are assumed to be rectangular with length $M|\vec{b}|$ and width $N|\vec{a}|$. The scattered intensity from a cluster is taken to be an incoherent sum of the intensities from each of its four facets. Figure 3a shows the resulting diffraction pattern at the diffraction conditions used to obtain the pattern shown in Fig. 2b. It can be seen that there is a 1:1 match between the observed and calculated diffraction patterns. The magnitude of the facet splitting relative to the substrate beams is set completely by the diffraction conditions, while the size and shape of the facet

beams are determined by the distribution of cluster sizes and shapes. Different facet structures give completely different patterns. For example, the diffraction pattern from a cluster with (117) facets is shown in Fig. 3b.

Figure 4 shows diffraction patterns for Ge clusters with (105) facets at diffraction conditions appropriate to reflection high-energy electron diffraction (RHEED). Patterns in two azimuthal orientations are shown. These two patterns illustrate the importance, in experiments, of changing the azimuthal direction of the incident-electron beam with respect to the substrate. In this example, changing the azimuth produces highly different patterns, from which the facet orientation can be identified. RHEED patterns from facets are most easily interpreted when the electron beam is directed along the steps or zone axes of the facet, as in Fig. 4a. Under such conditions diffraction from the facet 'rods' yields lines that clearly connect 3D diffraction features. The angle between these lines and the shadow edge defines the facet angle, the angle between the substrate surface and the facet. For electron-beam azimuths away from a facet's zone axis the projected angle between the facet 'rods' and shadow edge is less than the facet angle because of the way in which the Ewald sphere cuts these 'rods'. For example, it would be incorrectly concluded that the facet angle is 8.0° instead of 11.3° if measurements of (105) facets were made with the electron beam along [110] instead of along [100].

The metastable "hut" crystals appear to have been observed by others using RHEED[3]. Their measurements were, however, interpreted in terms of diffraction from 3D clusters having a structure suggested by Ourmazd and Bean.[4] This structure, consisting of alternating Si(111) and Ge(111) layers, yields a facet with a <110> zone axis. Such facets produce diffraction patterns that have no resemblance to these shown in Fig. 4; the experimental patterns[3] do, on the other hand, look like those shown in Fig. 4, suggesting that the phase observed by the authors of Ref. 3 is the same as ours. Although our calculations do not include multiple scattering, these effects cannot change the diffraction pattern in its essential features.

To our knowledge, this is the first time that a structure initially proposed on the basis of STM was subsequently confirmed by diffraction, rather than vice versa.

Acknowledgements

This work was supported by NSF, Solid State Chemistry Program, Grant No. DMR 89-15089 and is part by ONR, Chemistry Program. We would like to thank Don Savage for useful discussions and Mike Schacht for assistance.

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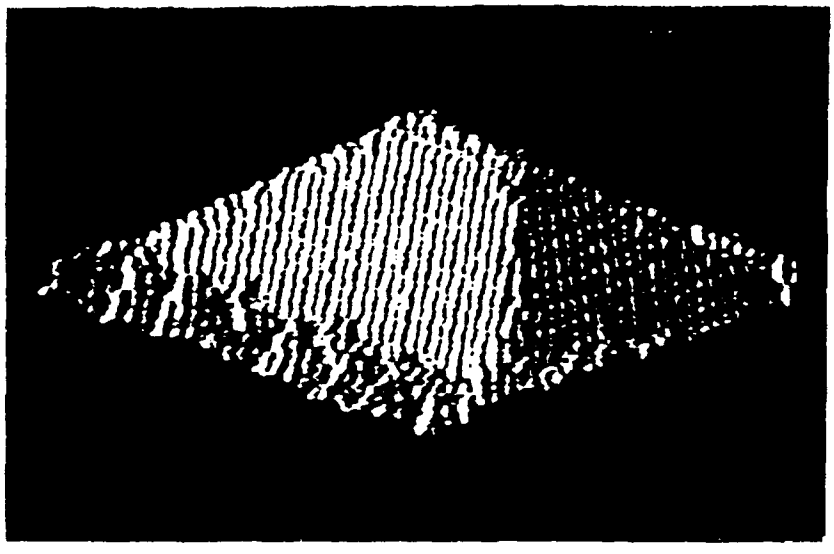
Figure Captions

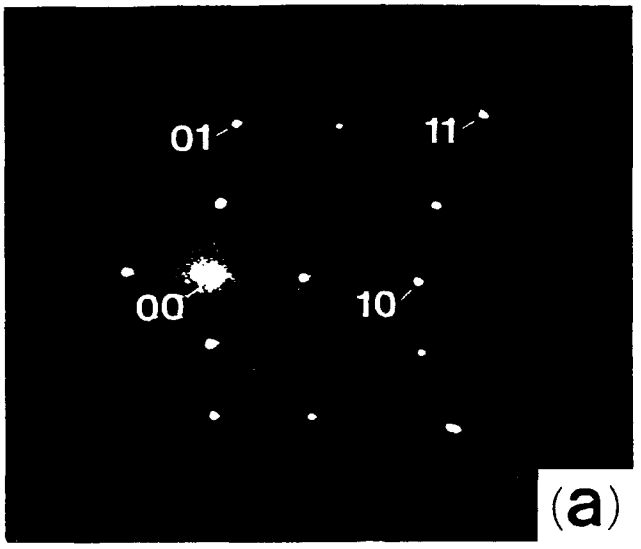
Fig. 1 STM image of a metastable Ge crystal. These crystals form on Si(001) for coverages >3 monolayers and for T < 800K. The crystallite is ∿30Å high and ∿200 Å long. From ref. 1.

Fig. 2 LEED patterns of clean and Ge-covered Si(001). a) LEED pattern of clean Si(001) showing a two-domain (2x1) diffraction pattern. Diffracted beams lie along [110]. b) LEED pattern showing the extra reflections from Ge crystallite facets, obtained with a ∿100eV beam at an angle of incidence of ∿80° measured from the horizontal, with the beam directed along [110].

Fig. 3 Simulated LEED pattern for clusters with two different facet orientations: a) {105} facets. b) {117} facets. {117} facets were used because they have a facet angle of 11.4°, which is very close to that of the {105} facets, but in a different orientation. The facet features for {117} facets are split in directions that are along lines connecting substrate beams. Both pictures are calculated at the diffraction conditions used in Fig. 2, assuming all clusters have the same size and (N,M) = (7,12) in Eq. (2).

Fig. 4 Simulated 20 KeV RHEED patterns for diffraction conditions satisfying the (004) reflection, with the beam directed along a) [100] and b) [110] for clusters with {105} facets. The (004) reflection at this energy occurs at an angle of incidence of 1.8°.

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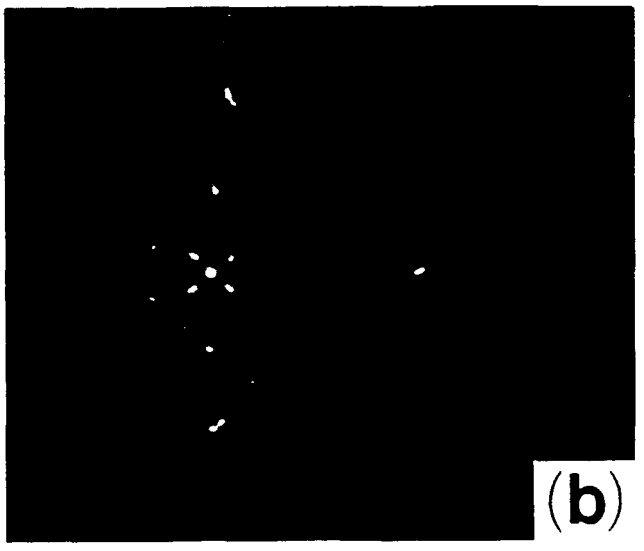
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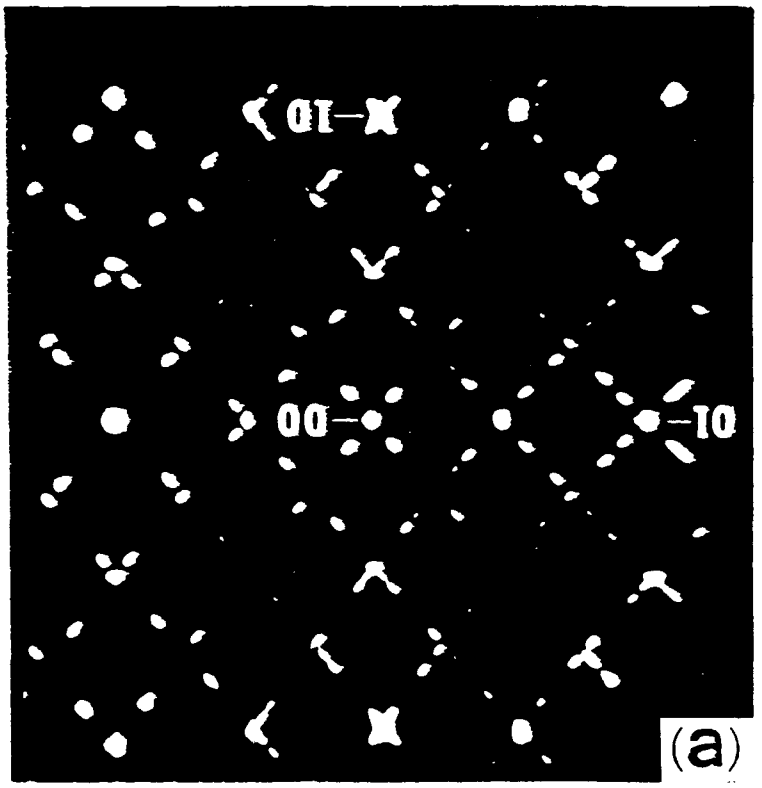
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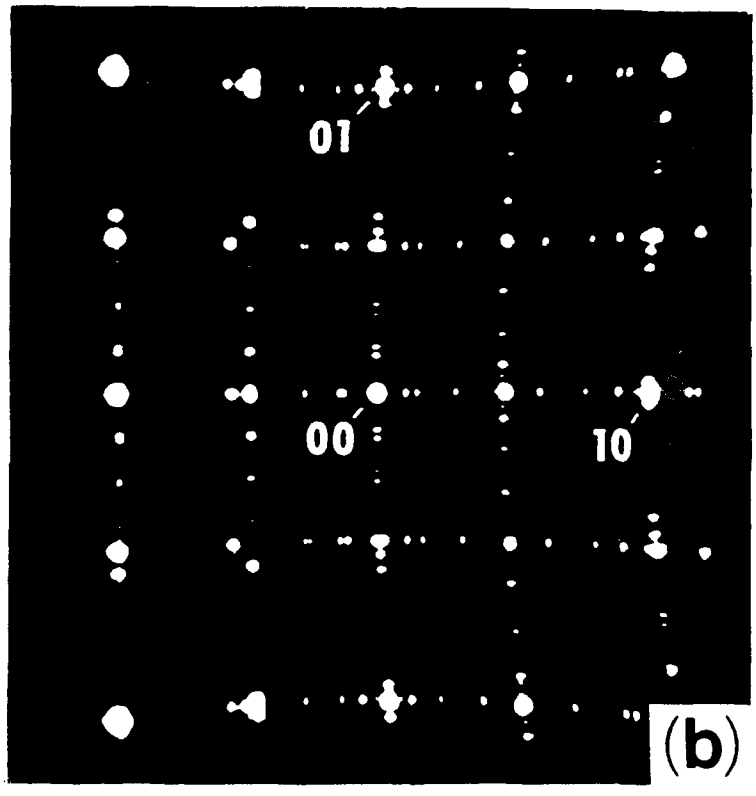
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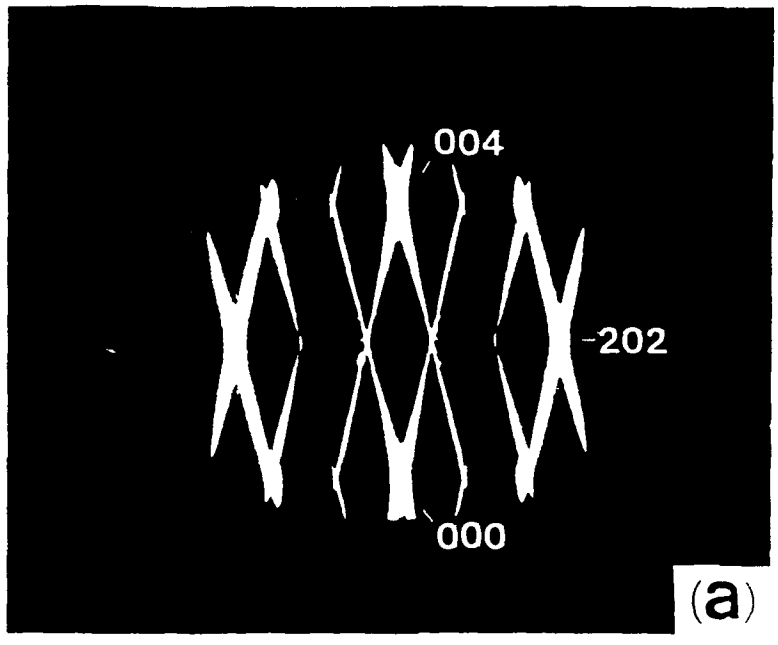
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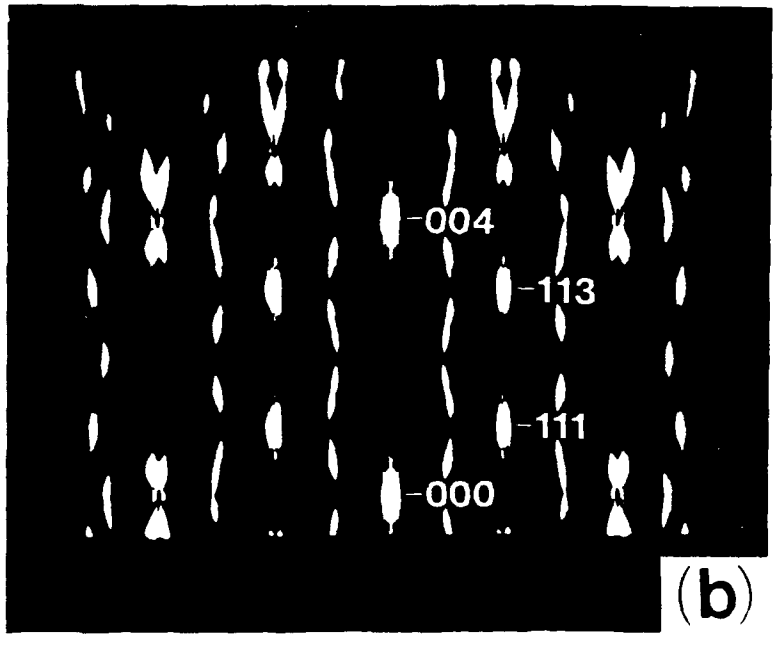
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